Quantum Mechanical Modeling of Ballistic MOS[illegible]

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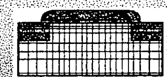
10/5/2001

Overview

- Develop theory, approximations and computer code to model quasi 1D structures such as nanotubes, DNA & MOSFETs*



- Nanotubes: Influence of defects on ballistic transport, Electro-mechanical properties, Metal-nanotube coupling
- DNA: Model electron transfer (biochemistry) and transport experiments, Sequence dependence of conductance
- MOSFETs: 2D doping profiles, Poly silicon depletion, Source to drain and Gate tunneling, Understand Ballistic limit

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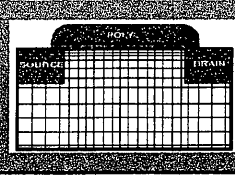
- **Similarities:**
- Source-drain, gate electrodes
- Layered structures
- Common structure for the Hamiltonian

$$\begin{bmatrix} h1 & U12 & & & \\ U21 & h2 & U23 & & \\ & U32 & h3 & U34 & \\ & & & & \\ & & & U & hm \end{bmatrix}$$

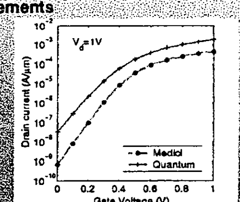
- Current transmission and electron density

- **Differences:**
- What are h & U?
- Tight-binding
- Huckel
- Quantum chemistry
- Effective mass
- Solving Poisson's equation



Outline

- What effects are modeled?
- Equations & computational requirements
- Specific Structures considered
- Drain current vs. Gate voltage of a well-tempered MOSFET



- Polysilicon depletion effect
- Ballistic? Transmission versus Energy
- Modeling of gate tunneling

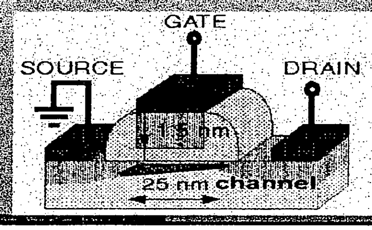
Model

Neglected:

- Discrete nature of dopant distribution
- Electron-impurity and electron-electron/phonon scattering
- n-MOSFETs
- Band-structure

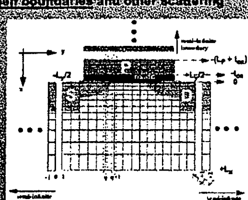
What do we model

- Anisotropic effective mass equation for electrons
- Carrier injection at source, drain and gate open boundaries
- Ballistic transport
- Source to Drain tunneling
- Gate Tunneling
- Non Equilibrium Green' function equations (Schrodinger-Poisson solver at finite biases)



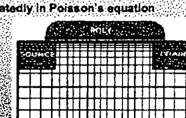
Equations

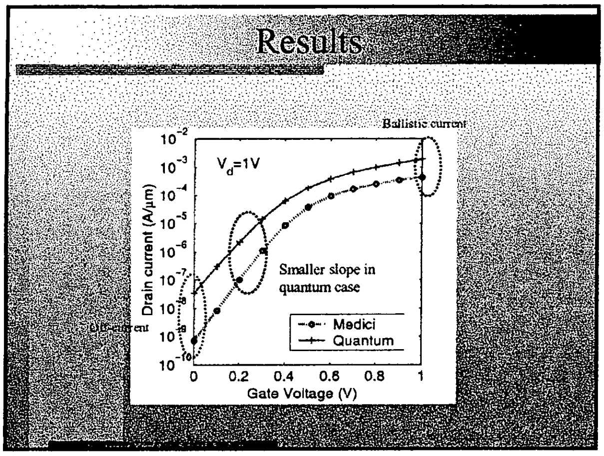
- Equations for retarded (Gr) and less-than (G<) Green's functions:
- $(E-H-\Sigma^r)\, G^r(r,r',E) = \delta(r-r')$
- $(E-H-\Sigma^r)\, G^<(r,r',E) = \Sigma^< G^a(r,r',E)$
- $(E-H-\Sigma^r)\, G^>(r,r',E) = \Sigma^> G^a(r,r',E)$
- Σ represents self-energy due to open boundaries and other scattering mechanisms
- $\Sigma = U\, g^r(\text{surface})\, U$
- Poisson's equation

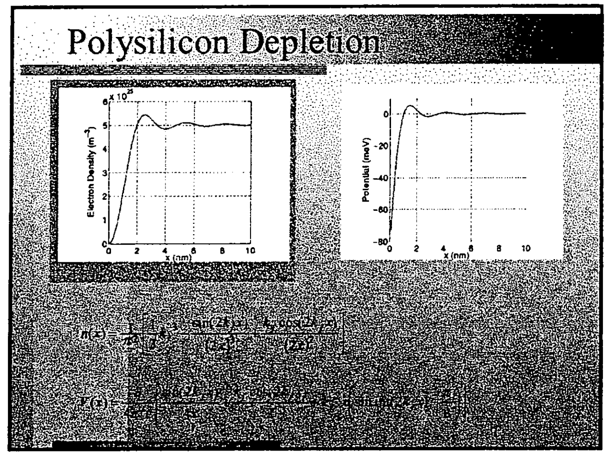


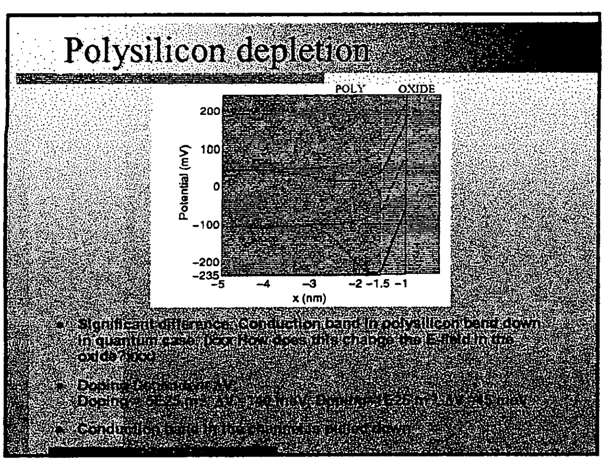
Computational requirements

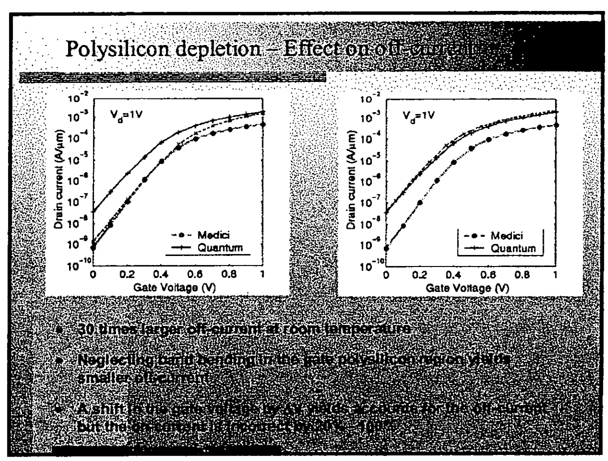
- $(E-H-\Sigma^r)\, G^<(r,r,E) = \Sigma^< G^a(r,r',E)$
- Electron density at r = $G^<(r,r,E)$ - Required repeatedly in Poisson's equation
- LHS is Block tridiagonal matrix
- Block size = Nx
- We require only the diagonal elements of $G^<$
- Developed an algorithm to solve for the diagonal blocks of $G^<$
- Number of operations= NE * Nx^3 * Ny
- NE – no. of energy grid points, (Nx,Ny) – no. of spatial grid points
- For Nx=75, Ny=350, 5E10 operations
- This is the bottleneck to realizing calculations with correct models of scattering [illegible]
- Challenge: To obtain the diagonal elements



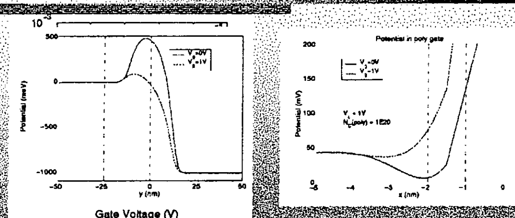

Results
Ballistic current
V_d=1V
Smaller slope in quantum case
Off-current
Medici
Quantum
Drain current (A/μm)
Gate Voltage (V)


Polysilicon Depletion
Electron Density (m^{-3})
x (nm)
Potential (meV)
x (nm)


Polysilicon depletion
POLY
OXIDE
Potential (mV)
x (nm)
Significant difference. Conduction band in polysilicon bend down in quantum case.
Conduction band in the channel is pulled down

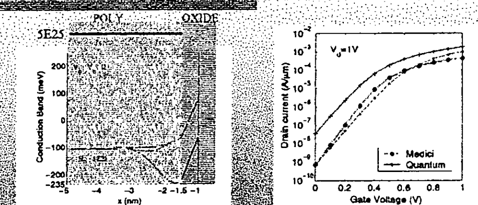

Polysilicon depletion – Effect on off-current
V_d=1V
Medici
Quantum
Drain current (A/μm)
Gate Voltage (V)
30 times larger off-current at room temperature
Neglecting band bending in the gate polysilicon region yields smaller off-current

Polysilicon depletion – Effect on on-current



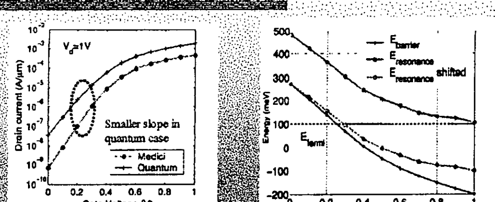
- Band bending in polysilicon gate depends on both gate bias and doping profile along y
- The source injection barrier moves towards the source by a large fraction of the channel length when a gate voltage is applied
- The conduction band near source injection barrier depends on both the doping profile along y and the gate bias
- A V_t shift by ΔV at Vg=1 overestimates on-current by 20% – 100%

Polysilicon depletion – Effect of tapered gate



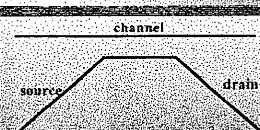
- At doping density of 5E25 m^{-3}, one dopant atom per $(1.3nm)^3$ box
- Some experimental reports that dopants near oxide may not be activated

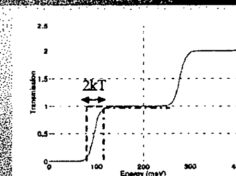
Resonant Levels

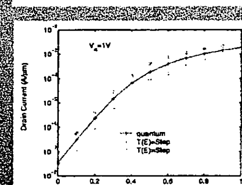


- Resonant levels decrease slower than barrier height with gate bias
- $E_{resonance}$ – Fermi level = few kT
- $I_{classical} \propto L_x \exp(-E_{barrier}/kT)$
- $I_{quantum} \propto L_x \exp(-E_{resonance}/kT)$

Transmission & Ballistic Transport

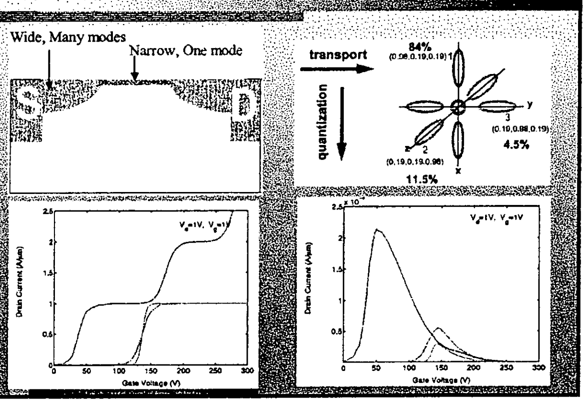






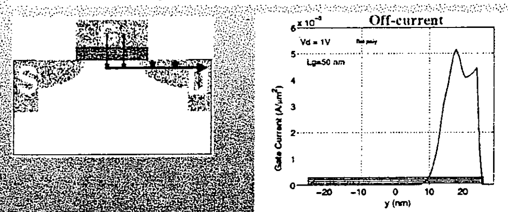
- Transmission is not unity at current carrying energies (*Even in the absence of scattering mechanisms.*)
- Significant errors in the estimate of on-current if a step function is assumed for Transmission versus energy
- Estimate gets worse with decrease in temperature

Anisotropic versus Isotropic effective mass



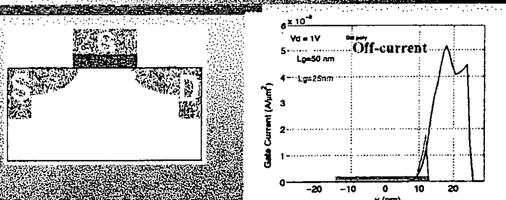
Gate Leakage

Gate leakage current = $\int dE\{T_{SG}(E)[F_S(E)-F_G(E)]+T_{DG}(E)[F_D(E)-F_G(E)]\}$

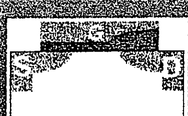


- Gate tunneling determines the off-current.
- Maximum gate tunneling current occurs at the gate-drain overlap region at zero bias.
- Can gate current be reduced without decreasing the on-current?

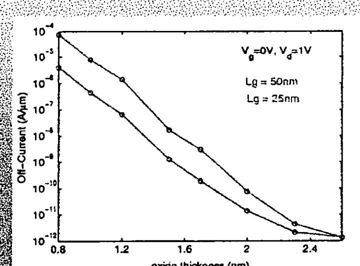
Gate Leakage – Polysilicon Gate Length (Lg)



- Off-current decreases by 20 times but on-current is to within 2% from Lg=50nm case.



Gate Leakage



Future Challenges:

- Increased role of tunneling and quantized levels in the channel of nanoscale MOSFET requires a better treatment of bandstructure
  - project underway: applying the 2D code to study transport in CNT with 4-orbital tight-binding Hamiltonian, which looks structurally the same
- Quantitative models for scattering are required
  - scattering time comparable to flight time
  - discretization of kz-space
- Hole band is required for pMOS
- Better algorithms are needed to solve NEGF equations
  - Need diagonal elements of Gr and G< rather than blocks